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Bayesian Determination of the Soil Hydraulic Parameters and the Time Validity of Philip’s Two-Term Infiltration Equation From Measured Infiltration Data

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Bayesian Determination of the Soil Hydraulic Parameters and the Time Validity of Philip's Two-Term Infiltration Equation From Measured Infiltration Data

by

Parakh Jaiswal

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Associate Professor Russell Detwiler

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Abstract

Bayesian Determination of the Soil Hydraulic Parameters and the Time Validity of Philip's Two-Term Infiltration Equation From Measured Infiltration Data

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University of California, Irvine

Associate Professor Jasper A. Vrugt, Chair

The topic of infiltration of water into variably saturated soils has received much attention in the soil physics literature in the past decades. Many different equations have been proposed to describe quantitatively the infiltration process. These equations range from simple empirical equations to more advanced deterministic descriptions of the infiltration process and semi-analytical solutions of Richards' equation. The unknown coefficients in these infiltration functions signify hydraulic properties and must be estimated by curve fitting to measured cumulative infiltration data, $\widetilde{I}(t)$.

From all available infiltration functions, the two-term equation, $I(t) = S\sqrt{t} + cK_\mathrm{s}t$ of Philip [1957] has found most widespread application and use. This popularity has not only been cultivated by detailed physical and mathematical analysis, the two-term infiltration equation is also easy to implement and admits a closed-form solution for the soil sorptivity, S ($\mathrm{L\,T}^{1/2}$), and multiple c ($-$) of the saturated hydraulic conductivity, K_s ($\mathrm{L\,T}^{-1}$). Yet, Philip's two-term infiltration function has a limited time validity, t_valid (T), and consequently, measured cumulative infiltration data, $\widetilde{I}(t)$, beyond $t = t_\mathrm{valid}$ (T) should not be used to estimate S and K_s (among others). The theoretical treatise in Philip [1957] provides a closed-form solution for the maximum time validity, t^+_valid, of the two-term infiltration equation. It is not particularly easy to experimentally corroborate these theoretical findings as this demands prior knowledge of c, S and K_s. What is more, the maximum time validity, t^+_valid may not characterize properly the actual time validity, t_valid. In this paper, we introduce a new method to determine simultaneously the values of the coefficient c, hydraulic parameters, S and K_s, and time validity, t_valid, of Philip's two-term infiltration equation. Our method is comprised of two main steps. First, we determine independently the soil sorptivity, S, and saturated hydraulic conductivity, K_s by fitting the semi-implicit infiltration equation of Haverkamp [Haverkamp et al., 1994] to measured cumulative infiltration data. This step uses the DiffeRential Evolution Adaptive Metropolis (DREAM) algorithm of Vrugt [2016] and returns as byproduct the marginal distribution of the parameter β in Haverkamp's infiltration equation. In the second step, the maximum likelihood values of S and K_s are used in Philip's two-term infiltration equation, and used to determine the optimal values of c and t_valid via model selection using the Bayesian information criterion. To benchmark, test and evaluate our approach we use cumulative infiltration data simulated by HYDRUS-1D [Simunek et al., 2008] for twelve different USDA soil types with contrasting textures. This allows us to determine whether our procedure is unbiased as the inferred S and K_s of the synthetic data are known before hand. Results demonstrate that the estimated values of S and K_s are in excellent agreement with their "true" values used to create the artificial infiltration data. Furthermore, our estimates of c and t_valid are dependent on soil texture and fall within the ranges stipulated in the literature.

Chapter 1

Introduction

Infiltration of water into variably-saturated soils is one of the most important and well studied processes in hydrology. Infiltration reduces (among others) flood risks, boosts water storage in the variably-saturated zone, replenishes reservoirs (aquifers), and helps alleviate land subsidence problems in areas that rely heavily on groundwater pumping as primary water source. Farmers in the Central Valley of California, for example, rely heavily on infiltration to maintain an adequate soil moisture status of the root zone in pursuit of an optimal crop yield.

If the supply rate of water to the soil surface is greater than the soil's ability to allow the water to enter, excess water will either accumulate on the soil's surface or runoff elsewhere following topographical gradients. Infiltrability is a term native to soil physics and hydrology that defines the maximum rate at which rain or irrigation water can be absorbed by a soil under given conditions. The infiltration rate thus determines how much water can enter the soil and which proportion of the rainfall or irrigation is expected to pond and end up as runoff or overland flow in lakes, streams, or rivers. Indeed, the infiltration rate of a soil exerts a large control on water availability and processes such as percolation, drainage, surface runoff, and evapotranspiration.

After the top soil has absorbed only some of the rainfall (or irrigation), the water moves further downward under the influence of gravity and/or capillary action soaking and/or filling up the pore space, replenishing the root zone, and possibly, seeping into rocks through cracks. In the past decades, a large number of models have been developed in the soil hydrology literature that describe quantitatively water infiltration into variably-saturated soils. These models or functions can be classified as empirical, semi-empirical or mechanistic. Empirical infiltration models are functions that were crafted by trial-and-error with the sole purpose of matching a laboratory of field measured time series of cumulative infiltration data. The resulting function may be viewed as a black-box relationship between cumulative infiltration, I (cm) and time t (h), which offers no insights into the underlying infiltration process nor provides evidence why the function would accurately portray the measured data. As a result, the parameters of empirical infiltration models are simply fitting coefficients whose values are difficult to interpret and relate to the underlying physical properties of the soil. Examples include the infiltration equations of Kostiakov [Kostiakov, 1932], Huggins and Monke [Huggins and Monke, 1966], modified Kostiakov [Smith, 1972], and Collis-George [Collis-George, 1977]. Semi-empirical infiltration models lie somewhere between deterministic infiltration models and their empirical (black box) counterparts. Such models enforce principles of mass balance (continuity equation), but the flux-concentration relationship that defines the connection between the infiltration rate, i ($\mathrm{cm\,h^{-1}}$), and cumulative infiltration, I (cm), is often hypothesized. Examples include the models of Horton [Horton, 1941], Holtan [Holtan, 1961], Singh [Singh and Yu, 1990], and Grigorjev [Grigorjev and Iritz, 1991]. Finally, the third and last group of infiltration models use a physically-based, reductionist, approach to describe the infiltration process. These models rely on mass conservation and Darcy's law to describe macroscopically soil water flow and storage. This includes the mechanistic models of Green and Ampt [Green and Ampt, 1911], Philip [Philip, 1957, 1969], Mein and Larson [Mein et al., 1971, Mein and Larson, 1973], Smith [Smith, 1972], Smith and Parlange [Smith and Parlange, 1978] and semi-implicit solution of Richards' equation of Haverkamp and coworkers [Haverkamp et al., 1994]. These models vary in complexity, depending in part on the resolved dimensionality, and choice of flow dynamics, unsaturated soil hydraulic conductivity function (hydraulic conductivity -

capillary head (or moisture content) relationship), soil water characteristic (retention function), and initial and boundary conditions.

From all work on infiltration, the work of Dr. John Philip (1927-1999) has probably received most attention and acclaim worldwide. While, he was recognized internationally for his contributions to the understanding of the movement of water, energy and gases, he is perhaps most known for his work on infiltration. His deep intuition of physical processes and excellent mathematical skills enabled him to make fundamental advances to the theory of infiltration. In his 1957 paper, Philip introduced the theory for one-dimensional infiltration into variably-saturated soils. In this paper he describes the cumulative infiltration, $I(t)$, as a finite (convergent) series as follows

$$\begin{aligned} I(t) &= a_1 t^{1/2} + a_2 t + a_3 t^{3/2} + \ldots + a_d t^{d/2} \\ &= \sum_{i=1}^{d} a_i t^{d/2}, \end{aligned} \tag{1.1}$$

where a_1 ($\mathrm{L\,T^{-1/2}}$) to a_d ($\mathrm{L\,T^{-d/2}}$) are soil dependent coefficients of the $d > 3$ expansion terms. Philip [1957] demonstrated that coefficient a_1 equates to the soil sorptivity, S ($\mathrm{L\,T^{-1/2}}$), and a_2 ($\mathrm{L\,T^{-3/2}}$) is an unknown multiple, c ($-$), of the saturated soil hydraulic conductivity, K_s ($\mathrm{L\,T^{-1}}$). Note that equation (1.1) is linear in its coefficients, $a_i; i = (1, \ldots, d)$. Consequently, we can use linear regression to determine in a single step the least squares values of the d coefficients and their underlying estimation uncertainty from measured cumulative infiltration data. Philip [1969] expressed the soil sorptivity as follows

$$S = \int_{\theta_\mathrm{i}}^{\theta_\mathrm{s}} \lambda(\theta)\mathrm{d}\theta, \qquad (1.2)$$

where θ_i ($\mathrm{L}^3\,\mathrm{L}^{-3}$) is the initial water content of the sample at the start of the infiltration experiment, θ_s ($\mathrm{L}^3\,\mathrm{L}^{-3}$) signifies the volumetric moisture content at saturation, and $\lambda(\theta)$ ($\mathrm{L}\,\mathrm{T}^{-1/2}$) is the Boltzmann variable

$$\lambda(\theta) = Z(\theta,t)t^{-1/2}, \qquad (1.3)$$

where $Z(\theta,t)$ is a so-called characteristic function which expresses the relationship between the depth, Z (L), in the soil column and the value of the volumetric water content, θ, at time $t \geq 0$ during an infiltration event under gravity-free conditions, where $\theta_\mathrm{i} \leq \theta \leq \theta_\mathrm{s}$.

In his seminal infiltration paper, Philip [1957] postulated that for $d \geq 3$ the coefficients, a_d, must satisfy

$$\frac{a_d}{S} > \left(\frac{a_2}{S}\right)^{d-1}. \qquad (1.4)$$

This condition promotes significance of the higher-order terms, but possibly at the expense of an erroneous approximation of $I(t)$ at large t. This is also known as Runge's phenomenon (polynomial wiggle) and cautions against the use of large d. The most popular variant of equation (1.1) uses only $d = 2$ expansion terms

$$I(t) = St^{1/2} + cK_\mathrm{s}t. \qquad (1.5)$$

This two-term formulation is easy to implement and use and has enjoyed widespread application and use among researchers and practitioners. This use is inspired in part by detailed physical and mathematical analysis of equation (1.5) by Philip and others. Nevertheless, the use of $d = 2$ expansion terms has a profound side-effect. As the higher-order expansion terms of equation (1.1) are discarded, Philip's two-term equation cannot describe adequately the infiltration at later times when the higher-order terms have an increasingly larger impact on the cumulative infiltration. In other words, Philip's two-term equation has a limited time validity, t_{valid} (T), and consequently, measured cumulative infiltration data, $\widetilde{I}(t)$, beyond $t = t_{\text{valid}}$ (T) should not be used to estimate the (least squares) values of S and K_{s}. Philip [1957] does provide a closed-form solution for the maximum time validity, t^{+}_{valid} (T), of the two-term infiltration equation,

$$t^{+}_{\text{valid}} = \left(\frac{S}{K_{\text{s}} - K_{\text{i}}} \right)^{2}, \tag{1.6}$$

at which gravity has the exact same impact on infiltration as capillary action. If $d > 2$ then Philip [1957] stipulates that t^{+}_{valid} increases with a factor of four. Philip [1957] coined this the characteristic time of the infiltration process, although we refer to it now as time validity, t^{+}_{valid}. Practical experience suggests, that it is not particularly easy to experimentally corroborate Philip's theoretical findings as this demands prior knowledge of c, S and K_{s}. What is more, the maximum time validity, t^{+}_{valid} may not characterize accurately the actual time validity, t_{valid}.

In this paper, we introduce a new method to determine simultaneously the values of the coefficient c, hydraulic parameters, S and K_{s}, and time validity, t_{valid}, of Philip's two-term infiltration equation. Our method is comprised of two main steps. First, we back out the soil sorptivity, S, and saturated hydraulic conductivity, K_{s} by fitting the semi-implicit infiltration equation of Haverkamp [Haverkamp et al., 1994] to measured cumulative infiltration data using the DiffeRential Evolution Adaptive Metropolis (DREAM) algorithm of Vrugt [2016]. The infiltration equation of Haverkamp is not particularly easy to use, but does not suffer a limited time validity, and instead can be used to simulate cumulative infiltration over the entire duration of the infiltration experiment. Our analysis, returns as byproduct the marginal distribution of the parameter β in Haverkamp's infiltration equation. This coefficient is directly related to the coefficient c in Philip's two-term infiltration equation according to $c = (2-\beta)/3$. In the second step, the maximum likelihood values of S and K_{s} are used in Philip's two-term infiltration equation, and used to determine the optimal values of c and t_{valid} via the Bayesian information criterion, or BIC. This information theoretic metric helps determine an optimal balance between the quality of fit of Philip's two-term infiltration equation and the length of the infiltration experiment. The BIC encodes a natural preference for simpler models. This parsimony principle is often attributed to

William of Ockham (1287-1347), an English Franciscan friar, scholastic philosopher, and theologian, but traceable to the works of philosophers such as Aristotle (384-322 BC) and Ptolemy (circa AD 90 to circa AD 168). and consistent with requirements of falsifiability in the scientific method of Popper [1992].

To benchmark, test and evaluate our approach we use cumulative infiltration data simulated by HYDRUS-1D [Simunek et al., 2008] for twelve different USDA soil types with contrasting textures. This allows us to determine whether our procedure is unbiased as the exact values of S and K_{s} are known before hand. The remainder of the paper is organized as follows. Section 2.1 introduces the measured cumulative infiltration data used herein to evaluate, test and benchmark our proposed two-step procedure. In Section 3 we detail the building blocks of of our methodology. Here, we are especially concerned with a description of Haverkamp's semi-implicit infiltration equation, the DREAM algorithm and the BIC for determination of the time validity, t_{valid} and the parameters c, S and K_{s} in Philip's two-term infiltration equation. This is followed in Section 4 with a preliminary discussion of the main results of our method. Finally, section 4.3 concludes the paper with a summary of our main findings.

Chapter 2

Materials and Methods

2.1 Measured infiltration data

To benchmark, test and evaluate the proposed method we need cumulative infiltration data and corresponding estimates of the sorptivity, S, and the saturated hydraulic conductivity, K_{s} of the soil column. These two hydraulic properties are of paramount importance in the present study as we are seeking an infiltration analysis method that provides accurate and unbiased estimates of S and K_{s}. Unfortunately, practical experience suggests that it is not particularly easy to accurately measure the soil sorptivity. This necessitates infiltration measurements under gravity-free conditions when water flow is largely controlled by capillary adsorption or desorption. This requires considerable experimental effort, particularly if we wish to evaluate our method for a large cohort of soils with contrasting textures. Therefore, we resort to synthetic infiltration data derived from numerical solution of Richards' equation using the Mualem-van Genuchten (MVG) [Mualem, 1976, Van Genuchten, 1980] soil hydraulic functions.

We used HYDRUS-1D [Simunek et al., 2008, 2016] to simulate cumulative infiltration into a homogeneous soil column of 200 cm depth for a period of 240 hours using a constant pressure head at the soil surface and free drainage condition at the bottom boundary of the profile. Table 2.1 lists the values of the MVG soil hydraulic parameter values that were used to create an infiltration data set for each USDA textural class. These parameter values originate from the HYDRUS-1D soil catalog [Carsel and Parrish, 1988].

As soil column discretization may affect the numerical results of HYDRUS-1D, simulated cumulative infiltration from a suite of different discretized profiles were compared against an analytic solution for infiltration without gravity, which is based on the Boltzmann transform. For each discretized profile, we plotted the simulated water content distribution in the soil column against the Boltzmann variable λ in Equation (1.2). A discretized profile is deemed accurate if the (θ, λ) relationships at many different simulation times coalesce in one single curve. The highest simulation accuracy was achieved for a discretized profile comprised of 401 nodes with a top

Table 2.1 Values of the Van Genuchten [1980] soil hydraulic parameters for the twelve USDA textural classes derived from Carsel and Parrish [1988]. The last two columns list the unsaturated soil hydraulic conductivity, $\widetilde{K}_s$, and sorptivity, $\widetilde{S}$, which are of main interest in the present study. The tilde operator is used for both variables to signify "measured" values. The value of $\widetilde{S}$ is computed with Eq. (1.2) using HYDRUS-1D simulated soil moisture values for a horizontal infiltration experiment.

Parameters	θ_r	θ_s	θ_r	α	n_{VG}	m_{VG}	$\widetilde{K}_s$	$\widetilde{S}$
	$cm^3\ cm^{-3}$			cm^{-1}	-	-	$cm\ h^{-1}$	$cm\ h^{-0.5}$
Clay	0.068	0.380	0.271	0.008	1.09	0.083	0.200	1.02
Clay loam	0.095	0.410	0.150	0.019	1.31	0.237	0.260	1.45
Loam	0.078	0.430	0.088	0.036	1.56	0.359	1.040	2.19
Loamy sand	0.057	0.410	0.057	0.124	2.28	0.561	14.592	6.20
Sand	0.045	0.430	0.045	0.145	2.68	0.627	29.700	9.21
Sandy clay	0.100	0.380	0.170	0.027	1.23	0.187	0.120	0.78
Sandy clay loam	0.100	0.390	0.111	0.059	1.48	0.324	1.310	1.60
Sandy loam	0.065	0.410	0.066	0.075	1.89	0.471	4.421	3.83
Silt	0.034	0.460	0.090	0.016	1.37	0.270	0.250	1.34
Silt loam	0.067	0.450	0.104	0.020	1.41	0.291	0.450	1.65
Silt clay	0.070	0.360	0.266	0.005	1.09	0.083	0.020	0.35
Silty clay loam	0.089	0.430	0.197	0.010	1.23	0.187	0.070	0.52

node of 10^{-6} cm and gradually decreasing spatial resolution downward in the soil column up to 1 cm depth for the bottom node.

To negate numerical errors and promote accuracy of the simulated cumulative infiltration curves, the internal interpolation tables of (θ, h) and (h, K) were disabled and the default initial time step of HYDRUS-1D was adjusted to satisfy convergence criteria for all different USDA soils. What is more, a modified MVG model with air-entry value of -2 cm was used for soils with $n_{VG} < 1.2$ to avoid unrealistically large changes in the hydraulic conductivity near saturation [Schaap and Van Genuchten,

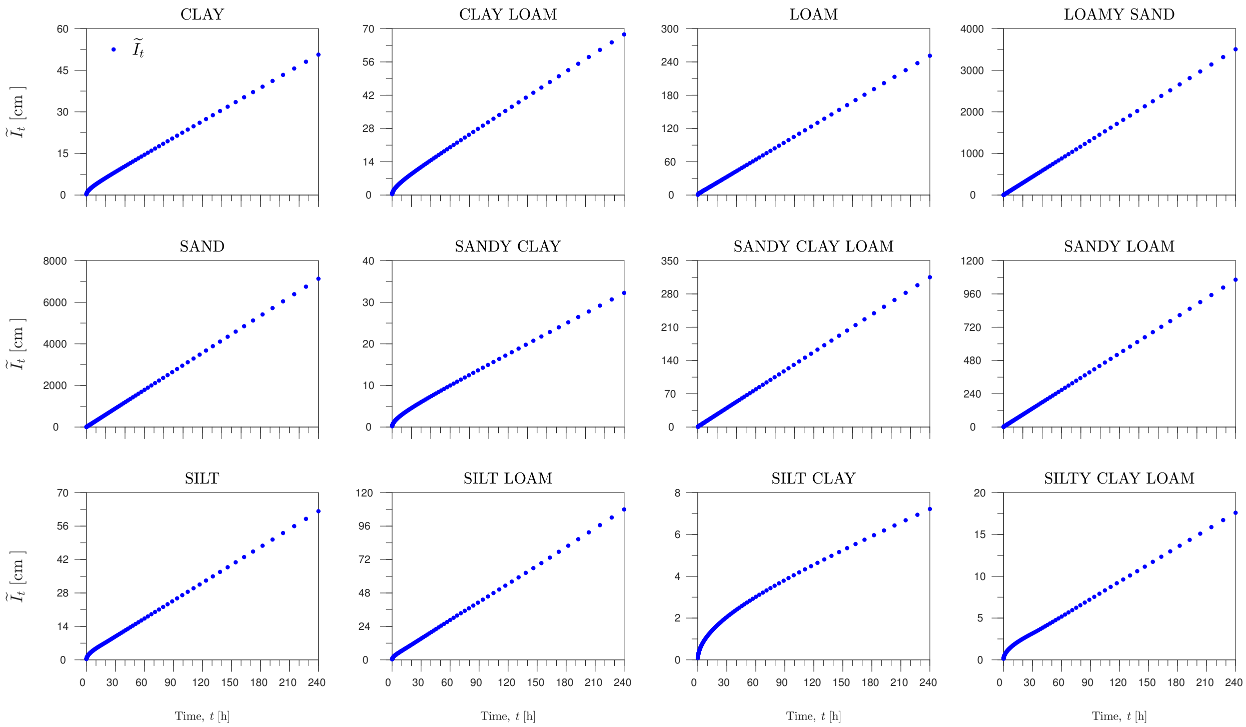

Figure 2.1 Given cumulative infiltration as a function of time for twelve USDA soils.

2006, Vogel and Cislerova, 1988, Vogel et al., 2000].

The infiltration data from the HYDRUS for the 12 USDA soils was for 240 hours. The time interval for the soils were different for different for each one. The total time interval was divided into 100 time points which were logarithmically distributed between 0 and 240 hours to maintain consistency. Figure 2.1 presents the infiltration curves for all soils with uniform time interval distribution. It is clear from the plots that amount of infiltration for the same time period varies significantly depending on the soil type. Cumulative infiltration in sand for 240 hours is 7130.4 cm while in clay it is 50.6 cm for the same time interval. Silty clay has lowest sorptivity and saturated hydraulic conductivity and thus the infiltration for the same amount of time is as low as 7.2 cm.

The infiltration data obtained was pre-processed as follows. For all the 12 soils the infiltration data was extracted up to 5 cm of infiltration. 5 cm was taken as the maximum infiltration here. 5 cm was used for all soils as it is the average minimum time for all the soils to give good estimate of the soil parameters. The data was then linearly interpolated to get a set of 100 data points. The corresponding time was interpolated which varied for different soils as different soils have different infiltration rates. This processed data will be used further for the estimation of the soil parameters.

Now we have discussed the measured infiltration data, we are left with estimation of the "true" soil sorptivity, S, for each USDA textural class. Unlike the saturated hydraulic conductivity, K_{s}, the soil sorptivity is not a parameter that is used in the MVG model. Rather, the sorptivity is a byproduct (e.g. function) of the MVG parameters θ_{s}, θ_{r}, α, n_{VG} and K_{s} listed in Table 2.1 and the initial moisture content, θ_{i}, of the 200 cm soil column. In theory, we can compute the value of S from the values of the MVG parameters. Yet, in practice this approach may not necessarily provide an accurate value of the sorptivity. Therefore, we resort to the formal definition of the sorptivity in Equation ((1.2)) and estimate the value of S using numerical integration of the $\lambda(\theta)$ curves simulated by HYDRUS-1D for infiltration without gravity. The last column in Table 2.1 reports the values of the sorptivity for each USDA textural class considered herein. This concludes the description of our data set.

Figure 2.2 and 2.3 display in a triangle plot the sorptivity and hydraulic conductivity values of the 12 USDA soils. These two figures show that $S_{\text{sand}} > S_{\text{silt}} > S_{\text{clay}}$ and $K_{\text{s sand}}$ $K_{\text{s silt}} > K_{\text{s clay}}$. As the hydraulic conductivity varies form 0.02 to 29.7 $\text{cm}\,\text{h}^{-1}$, we plot the logarithmic value of the hydraulic conductivity on the textural triangle. This will help make evident variability in the hydraulic conductivity values of the different soils.

Before we proceed to the next section, we store the HYDRUS-1D simulated cumulative infiltration data for each soil in a n-vector, $\{\widetilde{I}_1, \ldots, \widetilde{I}_n\}$ with corresponding (print) times $\{\widetilde{t}_1, \ldots, \widetilde{t}_n\}$ and measured values of the sorptivity and saturated hydraulic conductivity, $\widetilde{S}$ and $\widetilde{K}_{\text{s}}$, respectively. Thus, in the remainder of this paper, the tilde symbol is used to denote measured quantities.

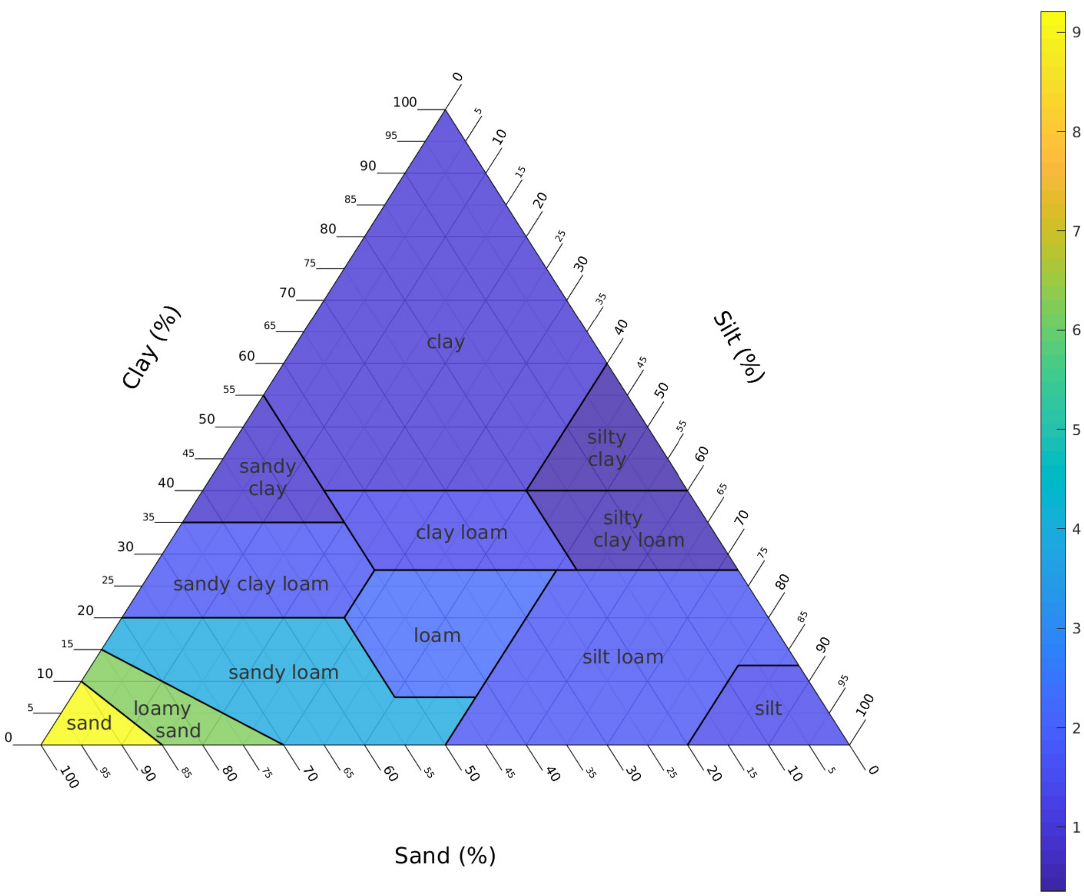

Figure 2.2 Soil Classification using true sorptivity(S) values.

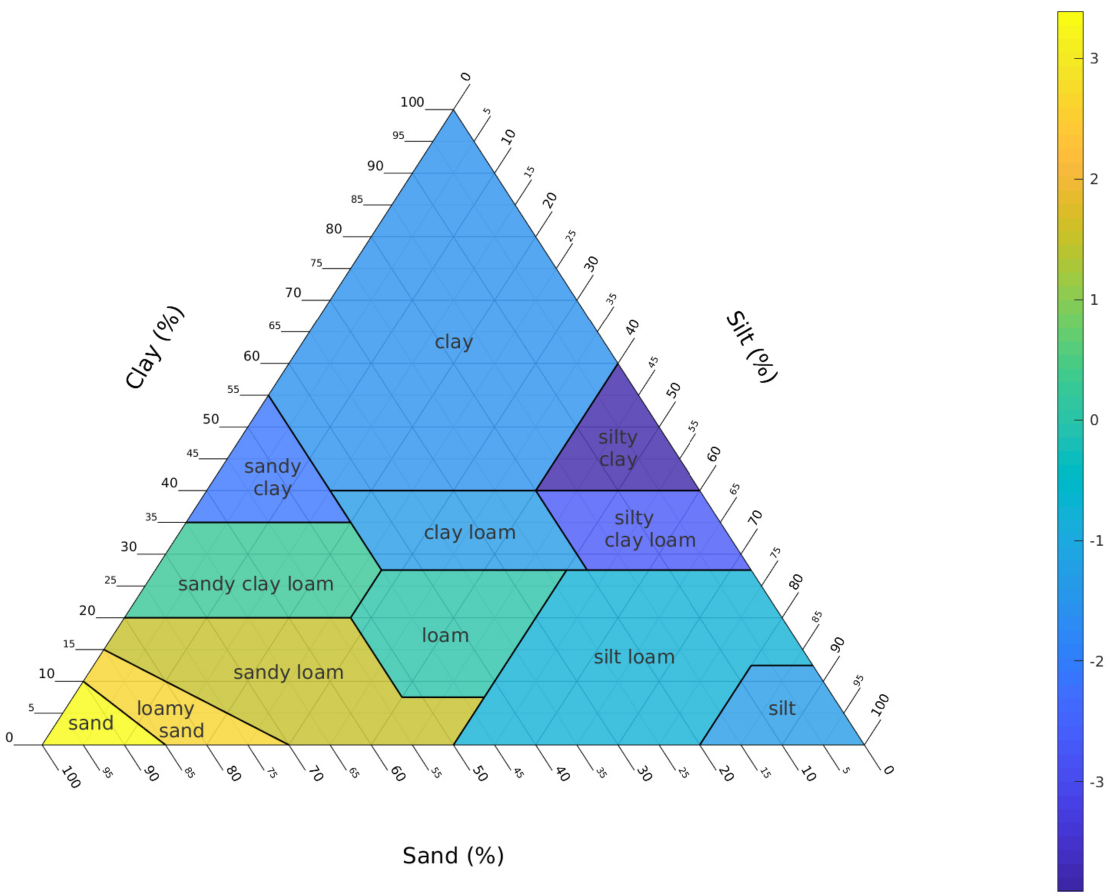

Figure 2.3 Soil Classification using true hydraulic conductivity($\log K_s$) values.

Chapter 3

Theory

In this section we describe the building blocks of our two-step procedure to determine the time validity, t_{valid} (L), of Philip's two-term infiltration equation (1.5) and the values of the unitless coefficient, c, soil sorptivity, S ($\mathrm{L\,T^{1/2}}$) and saturated hydraulic conductivity, K_{s} ($\mathrm{L\,T^{-1}}$).

3.1 Step 1: Haverkamp's semi-implicit infiltration equation

In a paper published in 1994 in Water Resources Research, Randel Haverkamp derived a quasi-exact analytic solution of Richard's equation to describe three-dimensional infiltration into variably-saturated soils [Haverkamp et al., 1994]. For a soil at uniform initial soil moisture content, K_i ($\mathrm{L\,T^{-1}}$), Haverkamp's equation can be used to predict vertical infiltration as follows

$$\frac{(K_\mathrm{s}-K_\mathrm{i})^2}{S^2}(1-\beta)t = \frac{(K_\mathrm{s}-K_\mathrm{i})I}{S^2} - \frac{1}{2}\log\left\{\frac{1}{\beta}\exp\left[\frac{2\beta(K_\mathrm{s}-K_\mathrm{i})I}{S^2}\right]+\frac{\beta-1}{\beta}\right\}, \quad (3.1)$$

where β is a unitless parameter that primarily affects the shape of the simulated cumulative infiltration curve, $I(t)$, at late times, and t denotes time (T). The value of β is defined as follows [Haverkamp et al., 1994]

$$\beta = 2 - 2\,\frac{\int\limits_{\theta_\mathrm{i}}^{\theta_\mathrm{s}} \left(\frac{K-K_\mathrm{i}}{K_\mathrm{s}-K_\mathrm{i}}\right)\left(\frac{\theta_\mathrm{s}-\theta_\mathrm{i}}{\theta-\theta_\mathrm{i}}\right) D_\mathrm{w}(\theta)\mathrm{d}\theta}{\int\limits_{\theta_\mathrm{i}}^{\theta_\mathrm{s}} D_\mathrm{w}(\theta)\mathrm{d}\theta}, \quad (3.2)$$

where θ ($\mathrm{L^3\,L^{-3}}$) is the soil moisture content of the sample at time t after the start of the experiment, $\theta_\mathrm{i} \leq \theta \leq \theta_\mathrm{s}$, and $D_\mathrm{w}(\theta)$ ($\mathrm{L^2\,T^{-1}}$) is the so-called soil water diffusivity function.

A theoretical treatise of three-dimensional infiltration from a disc infiltrometer by Smettem et al. [1994] established a mathematical relationship between the coefficient a_2 in Philip's cumulative infiltration expansion of equation (1.1) and the pressure head, h_0 (L) and radius, r_0 (L), of the disc infiltrometer, and the hydraulic conductivity, $K(h_0)$ of the surrounding soil at h_0 as follows

$$a_2 = \frac{(2-\beta)K(h_0}{3} - \frac{\gamma S^2}{r_0(\theta(h_0)-\theta_\mathrm{i})}, \quad (3.3)$$

where γ is a unitless proportionality constant assumed to be in between 0.6 and 0.8, and $\theta(h_0)$ ($L^3\,L^{-3}$) is the volumetric moisture content at h_0. The work of Smettem et al. [1994] also confirmed that coefficient a_1 in equation (1.1) equates to the soil sorptivity, S.

Past publications by Haverkamp and co-workers have shown that their semi-implicit solution of Richards' equation in (3.1) is in excellent agreement with measured cumulative infiltration data from a range of different soils. What is more, unlike Philip's two-term formulation in equation (1.5), the so-called Haverkamp equation does not suffer a limited time validity. Instead, equation (3.1) is valid over the entire duration of the infiltration experiment. The excellent fit to experimental data and long-term validity of equation (3.1) are desirable qualities, nonetheless, this did not convince soil hydrologists to adopt Haverkamp's equation for infiltration data analysis and interpretation in lieu of Philip's two-term equation. The explanation is as simple as discouraging. As Haverkamp's equation is a semi-implicit solution, most researchers and practitioners experience problems with numerical solution of $I(t)$. This is evident if we study in detail equation (3.1). At each time t, the value of the cumulative infiltration I needs to be determined iteratively so that the left-hand-side of equation 3.1 matches exactly the value on its right-hand side.

To simplify the application of equation (3.1), Haverkamp et al. [1994] derived three explicit solutions for the cumulative infiltration at very short (VS), short (S), and long (L) times, respectively. The resulting equations are listed below

$$I^{\mathrm{VS}}(t) = S\sqrt{t} \tag{3.4a}$$

$$I^{\mathrm{S}}(t) = S\sqrt{t} + \left[\left(\frac{2-\beta}{3}\right)\Delta K + K_{\mathrm{i}}\right] t \tag{3.4b}$$

$$I^{\mathrm{L}}(t) = K_{\mathrm{s}}t + \frac{1}{2(1-\beta)}\frac{S^2}{\Delta K}\log\left(\frac{1}{\beta}\right). \tag{3.4c}$$

Time limits for the approximate validity of the three different equations were developed by Lassabatere et al. [2009], including their dependency on soil textural class. Yet, these time limits cannot be calculated analytically, and instead we must resort to numerical computation. In the same paper, Lassabatere et al. [2009] demonstrated that the use of a soil specific β value, estimated from soil textural data, can improve simulation accuracy of the infiltration process and hence the estimation of K_{s} and S from infiltration data.

The three explicit solutions listed in equations (3.4a) - (3.4c) are of great practical value for simulating vertical infiltration. Yet, this demands prior knowledge of the sorptivity, S, saturated hydraulic conductivity, K_{s} and β value of the soil column. This equates to an inverse problem wherein the measured cumulative infiltration curve is used to back out the values of the three soil parameters. Yet, as there is no direct way of determining the time validity of the three listed expressions, we should use instead the semi-implicit solution of equation (3.1). We resort to a root finding algorithm to automatize the solution of $I(t)$. At each time, t, we can use Newton's method to solve for the cumulative infiltration, I. Appendix A provides a MATLAB recipe of our root finding procedure. This code uses as input arguments a n-vector of time values and a 1×3 vector of parameter values, S, K_{s} and β and returns to the user a $n \times 1$ vector with simulated cumulative infiltration values according to Haverkamp's infiltration equation 3.1.

In the past few years, Haverkamp's infiltration equation has steadily received more and more interest in the vadose zone community. As equation 3.1 can describe accurately measured cumulative infiltration curves, and is valid over the entire duration of the infiltration experiment, we use it herein to back out the values of the soil sorptivity, S, saturated hydraulic conductivity, K_{s} and β. This amounts to inverse modeling and necessitates the use of a parameter estimation algorithm.

Before we proceed to a description of the DREAM algorithm we first revisit Haverkamp's infiltration equation. If we make the convenient assumption that the hydraulic conductivity, K_{i}, at the initial moisture content, θ_{i}, equates to zero, then equation (3.1) simplifies to

$$\left(\frac{K_{\mathrm{s}}}{S}\right)^2 (1-\beta)t = \frac{K_{\mathrm{s}} I}{S^2} - \frac{1}{2}\log\left\{\frac{1}{\beta}\exp\left[\frac{2\beta K_{\mathrm{s}} I}{S^2}\right] + \frac{\beta - 1}{\beta}\right\}, \tag{3.5}$$

This reduces the number of unknown parameters to three, namely, S, K_{s} and β. This simplification is not given in by limitations of our parameter estimation algorithm as the Bayesian approach used herein can easily handle a very large number of parameters. A comparison of the marginal distribution of each parameter with its prior distribution would convey the amount of available information in the cumulative infiltration data to constrain each parameter. Instead, we use equation 3.5 as we anticipate that in most cases we may not know exactly the initial moisture content, θ_i of the sample, let alone its corresponding hydraulic conductivity. Nevertheless, the use of equation 3.5 should be acceptable for infiltration experiments with an initially dry sample. Then, θ_i is rather small and $K(\theta_\mathrm{i}) \ll K_\mathrm{s}$ and close to zero.

This paper is not the first attempt to inversely estimate the values of S, K_s and *beta* in Haverkamp's infiltration equation. For example, Latorre et al. [2015] used equation 3.1 to estimate the soil sorptivity, S, and saturated hydraulic conductivity, K_s from measured cumulative infiltration curves. But they set $\beta = 0.6$ based on recommendations in Haverkamp et al. [1994]. they d Dohnal et al. [2010] simulated infiltration curves in which he used the Haverkamp et al. [1994] and Zhang [1997] model to get sorptivity and hydraulic conductivity and then used it to get the infiltration curves from the Philip [1957]'s model.

Table 3.1 DREAM_ZS prior information of parameters.

Parameters	Minimum	Maximum
S cm h$^{-0.5}$	0	10
K_s cm h^{-1}	0	50
β	0	5

3.2 Step 1: The DiffeRential Evolution Adaptive Metropolis (DREAM) algorithm

To estimate the parameters in Haverkamp's infiltration equation (3.5) we use Bayesian inference with the DREAM algorithm. A detailed description of this method appears in Vrugt [2016], and interested readers are referred to this paper for more information. The DREAM algorithm is a general-purpose parameter estimation algorithm which has found widespread application and use in fields ranging from physics, chemistry and engineering, to ecology, hydrology, and geophysics. In the present application we assume uniform prior distributions for the parameters S, K_s and β with ranges listed in Table 3.1.

Note, that equation (3.2) implies a maximum value of β of two. In our prior distribution listed in Table 2, we allow for values of β larger than two. This may seem awkward but is done purposely to test the robustness of our procedure. As we will show later, the value of β is larger than two for the sandy clay loam and silty clay loam soils. Despite this apparent inconsistency, the values of S and K_s of those soils appear in close agreement with their "measured" counterparts.

A Gaussian likelihood function was deemed appropriate to determine the posterior distribution of the parameters

$$L(\mathbf{x}|\widetilde{\mathbf{I}}) \propto \left(\sum_{j=1}^{n} \left(\widetilde{I}(\tilde{t}_j) - I(\mathbf{x}, \tilde{t}_j) \right)^2 \right)^{-\frac{n}{2}}, \tag{3.6}$$

where $\mathbf{x} = \{ S, K_\mathrm{s}, \beta \}$ is our 1×3 vector with parameter values of equation (3.5), $\tilde{I}(\tilde{t}_j)$ denotes the measured cumulative infiltration at the j^{th} measurement time and $I(\mathbf{x}, \tilde{t}_j)$ signifies the predicted cumulative infiltration with equation 3.5 at time $\tilde{t}_j$ using the parameter values, $\mathbf{x}$. The posterior density now equates to the product of the prior density and the likelihood. Note, that the term within the brackets equates to the sum of squared residuals used commonly in curve fitting. Convergence of the sampled chain trajectories to the posterior distribution is monitored with a suite of different convergence statistics. We use the last 25% of the samples in each chain to summarize the posterior distribution of the parameters.

3.3 Step 2: Estimation of c and t_{valid} in Philip's two-term equation

The posterior distribution of the soil sorptivity, S, saturated hydraulic conductivity, K_{s} and coefficient β in Haverkamp's infiltration model serves as input to our second step. We isolate the maximum likelihood solution from the Markov chains sampled with the DREAM algorithm, and use these values "as is" in Philip's two-term infiltration equation. This leaves us with two unknowns for each soil, the unitless coefficient c and the time validity, t_{valid} of equation 1.5. As Philip's two-term equation is linear in c, we can use linear regression to determine its optimal value for any subset of cumulative infiltration measurements. Once this value is known we can compute the likelihood of c using equation 3.6. For each soil we follow the following procedure to determine the time validity, t_{valid}

1. Take the maximum likelihood values of S and K_{s} derived from the DREAM algorithm and enter those in equation (1.5).

2. Start with the third measured cumulative infiltration value, $j = 3$

3. Determine the least squares value of c via linear regression.

4. Compute the likelihood of c using equation (3.6)

5. Compute the BIC metric.

$$BIC(k, j) = -2\log\big(L(c|\widetilde{\mathbf{I}})\big) + k\ln j, \tag{3.7}$$

   where $k = 1$ is the number of parameters that is estimated in Philip's two-term infiltration equation.

6. As long as j is smaller than n, set $j = j + 1$ and go back to step 3. Otherwise, stop

Now we can inspect the $n - 2$ values of BIC to determine the time validity of Philip's two term infiltration equation. The "model" with minimum value of the BIC is preferred statistically. Thus, we pick the length of the data set, j that has the smallest value of the BIC. The corresponding time defines the value of t_{valid}. As the length of the time series is increased incrementally, we have to use a metric such as the BIC to determine the time validity of equation (1.5).

Chapter 4

Results

4.1 Results from Haverkamp's equation

The results for the twelve soils are presented in the Table 4.1. This shows the optimum values of the three parameters S, K_S and β from the DREAM_ZS. As seen in the table the estimates are pretty close to the ”true” values for all the three parameters.

Figure 4.1 and 4.2 show the posterior distribution of S and K_s from DREAM. We can see that the posterior is well defined and the standard deviations are low for all the soils. The red cross denotes the optimum values for each soil.

Table 4.2 lists the statistics of the DREAM posterior. The 95% credible values for clay soil lies between 1.0281 and 1.0319 which is a reasonable estimate given a uniform

Table 4.1 DREAM_ZS optimum results for the parameters.

Parameters	$\widetilde{S}$	$\widetilde{K}_{\mathrm{s}}$	β
	cm $\mathrm{h}^{-0.5}$	cm h^{-1}	
Clay	1.0308	0.2101	1.5219
Clay loam	1.4789	0.2938	1.3584
Loam	2.2458	0.9496	1.3922
Loamy sand	6.2492	15.0777	0.7550
Sand	9.2280	31.2837	0.6115
Sandy clay	0.7914	0.1336	1.2541
Sandy clay loam	1.7859	1.2705	2.4816
Sandy loam	3.8653	4.3761	0.9548
Silt	1.3702	0.1935	1.6050
Silt loam	1.6895	0.3642	1.5533
Silt clay	0.3503	0.0204	1.5793
Silty clay loam	0.5930	0.0631	3.8077

Table 4.2 Statistics of DREAM posterior for twelve soils.

Soils	S (cm $\mathrm{h}^{-0.5}$)				K_{s} (cm h^{-1})			
	2.5%	Mean	Median	97.5%	2.5%	Mean	Median	97.5%
Clay	1.0281	1.0305	1.0313	1.0319	0.2097	0.2102	0.2102	0.2107
Clay loam	1.4748	1.4779	1.4780	1.4802	0.2858	0.2909	0.2930	0.2949
Loam	2.2444	2.2467	2.2470	2.2484	0.9477	0.9513	0.9515	0.9540
Loamy sand	6.2363	6.2428	6.2417	6.2489	15.0167	15.0334	15.0264	15.1249
Sand	9.2017	9.2296	9.2326	9.2548	31.0992	31.2836	31.2905	31.4710
Sandy clay	0.7870	0.7895	0.7892	0.7 936	0.1284	0.1327	0.1327	0.1376
Sandy clay loam	1.7556	1.7844	1.7839	1.8082	1.2668	1.2703	1.2705	1.2734
Sandy loam	3.8569	3.8765	3.8739	3.9201	4.3414	4.3937	4.3912	4.4809
Silt	1.3688	1.3705	1.3705	1.3721	0.1902	0.1929	0.1928	0.1955
Silt loam	1.6880	1.6906	1.6910	1.6929	0.3634	0.3668	0.3667	0.3703
Silt clay	0.3471	0.3516	0.3516	0.3567	0.0195	0.0205	0.0198	0.0217
Silty clay loam	0.4995	0.5363	0.5273	0.5930	0.0555	0.0596	0.0589	0.0633

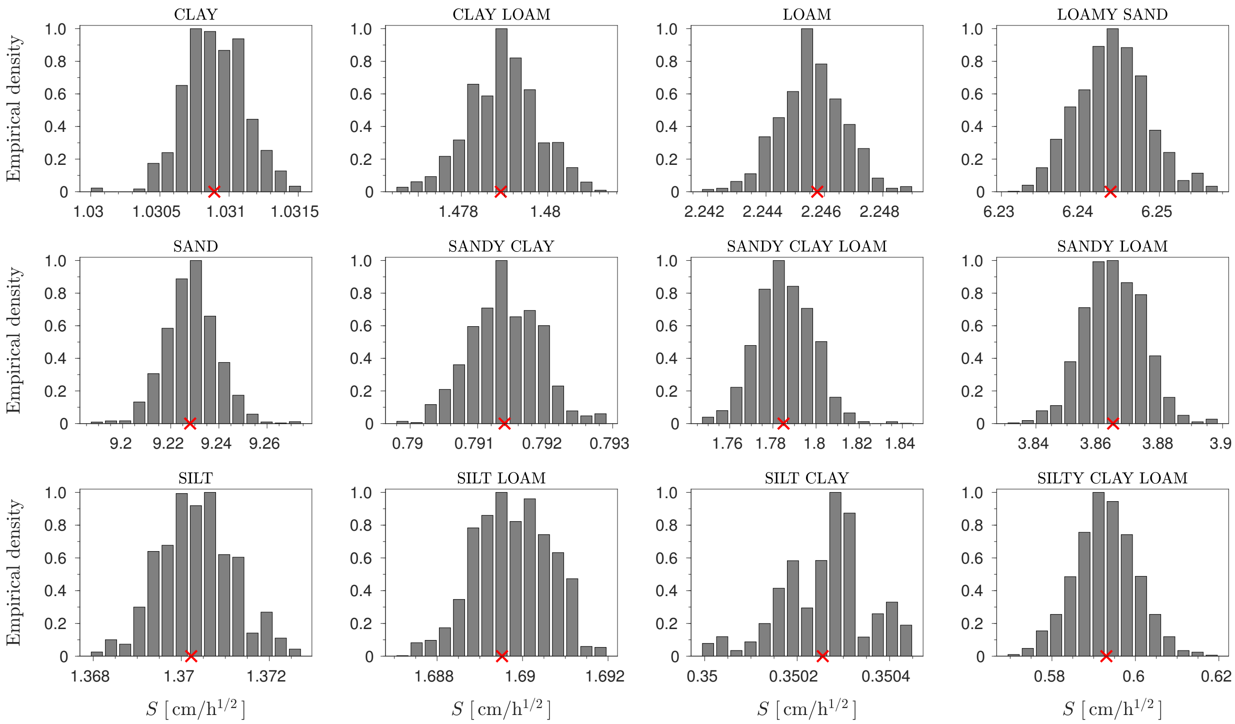

Figure 4.1 Histogram of DREAM derived posterior distribution of Sorptivity.

prior from 0 and 10 cm $h^{-0.5}$.

Figure 4.3 represents the accuracy of the estimated and "true" parameters. This plot shows the "true" and estimated values of S and K_S. A line of unity is drawn to see the accuracy of the estimation. The values lie on the line of unity. This scatter plot verifies that the estimated parameters are close to the "true" values and we can estimate the parameters accurately from cumulative infiltration data up to 5 cm using the Haverkamp's equation.

The β parameter predicted lies within zero and two for all the soils except sandy clay

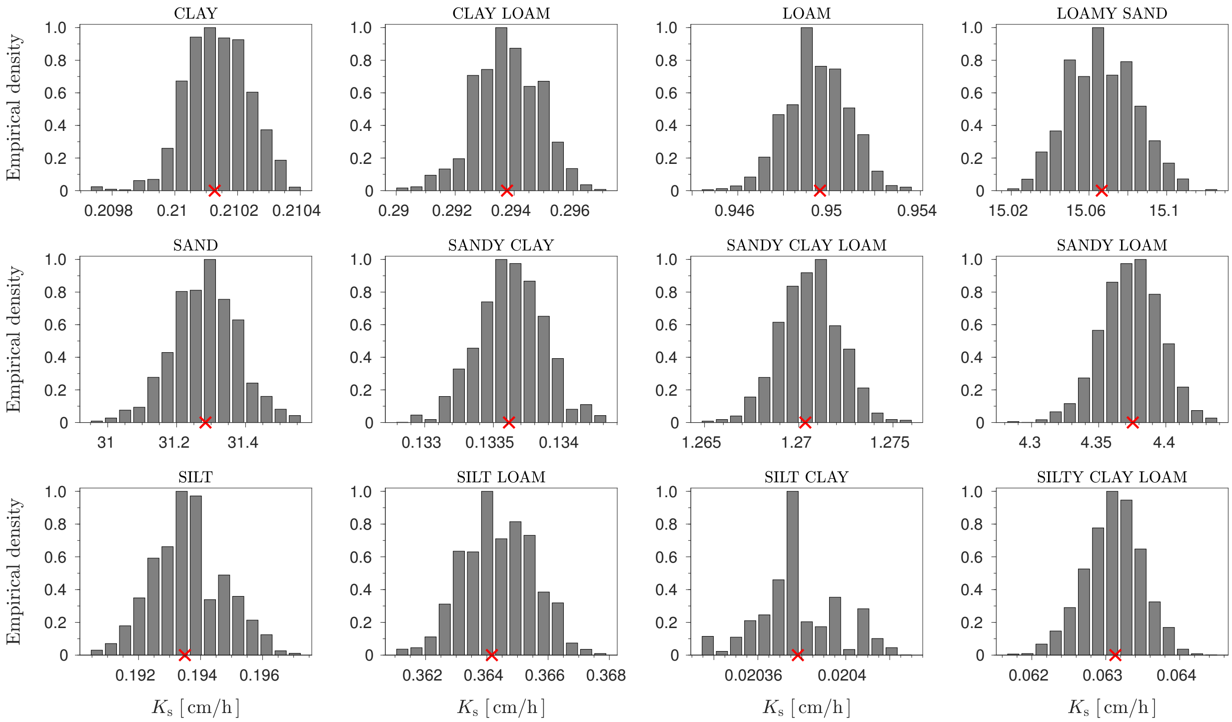

Figure 4.2 Histogram of DREAM derived posterior distribution of Hydraulic conductivity.

Table 4.3 Correlation table.

Parameters	S,K_s	K_s,β	β,S
Clay	0.8137	0.9642	0.9347
Clay loam	0.8699	0.9574	0.9737
Loam	0.8508	0.9651	0.9557
Loamy sand	0.8414	0.9533	0.9632
Sand	0.8214	0.9265	0.9742
Sandy clay	0.8384	0.9570	0.9579
Sandy clay loam	0.5955	0.9877	0.6995
Sandy loam	0.8276	0.9530	0.9562
Silt	0.9021	0.9710	0.9774
Silt loam	0.8760	0.9659	0.9689
Silt clay	0.8473	0.9691	0.9486
Silty clay loam	0.6553	0.9869	0.7538

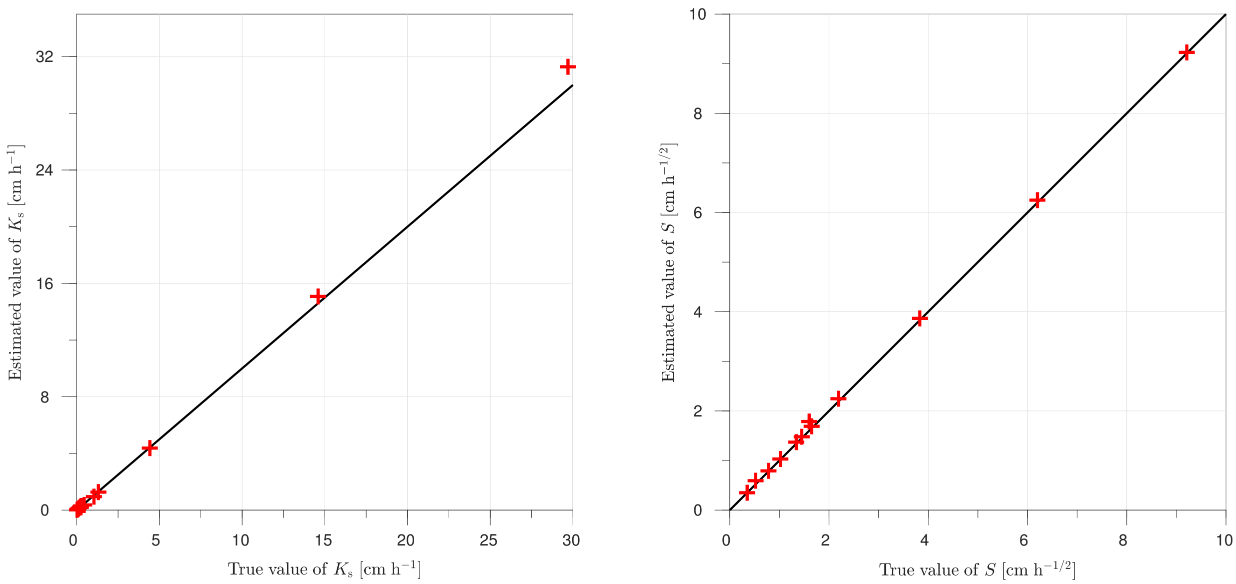

Figure 4.3 Scatter plot of true and estimated S and K_s using Haverkamp's equation with 5 cm of infiltration.

loam and silty clay loam. When we bound the parameters to two the sorptivity and hydraulic conductivity are also affected by the change and they estimate slightly lower values than the ”true” parameter values. The correlation is later shown in the table 4.3 for the three parameters. The values for these two soils show that the correlation between K_s and β is higher as compared to the correlation between K_s and S or the correlation between S and β. Thus, changes in the β values for these two soils will most likely affect the estimation of the hydraulic conductivity values.

To check that the estimated parameters can be used in Eq. 3.1, we plot Figure 4.4 which shows the predicted infiltration from the Haverkamp's equation using the

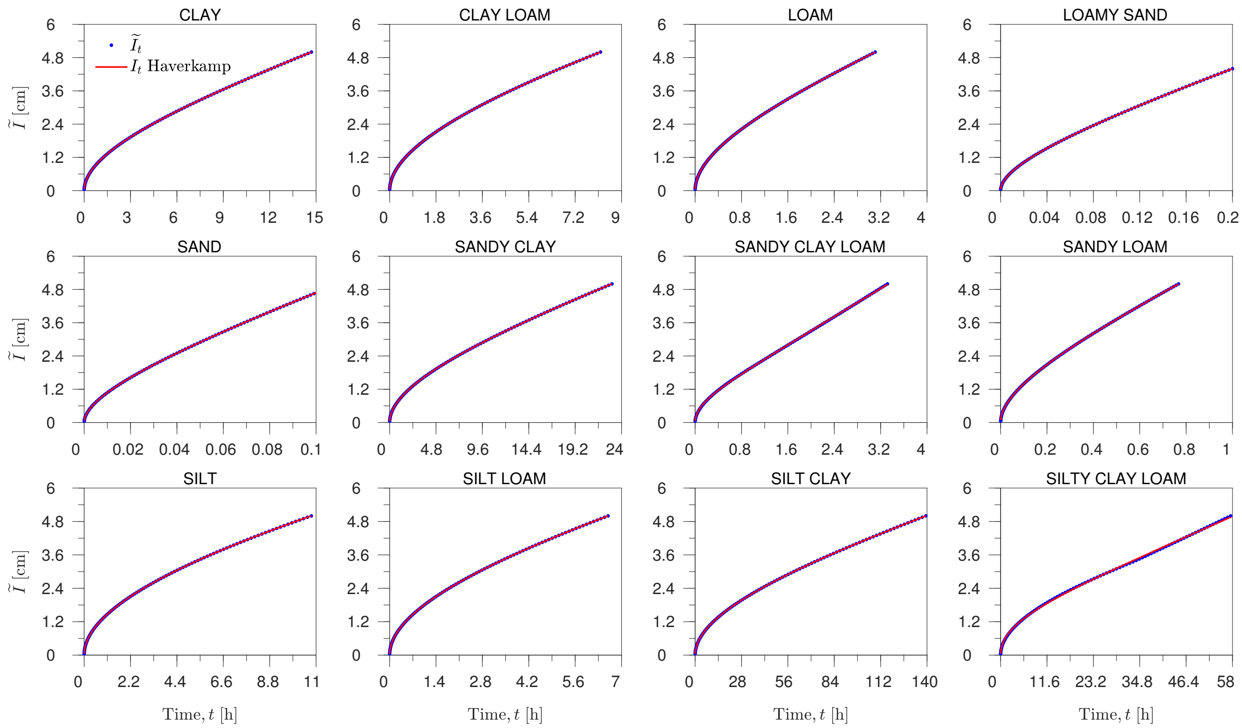

Figure 4.4 Cumulative infiltration as a function of time using Haverkamp's equation with estimated values of S and K_s.

DREAM estimated S, K_s and β. The predicted infiltration values are compared with the original infiltration data up to 5 cm. Figure 4.4 shows that the predicted values are a good match for all the soils. The only slight deviation is in the silty clay loam.

Further analysis was done to see the textural relation of the shape parameter β. Figure 4.5 shows the estimated β values plotted on soil textural triangle. The β values for sandy clay loam and silty clay loam are higher than all other soils. The β values for these two soils are higher than two. Previous literature presents that the β value should be less than 2 but for these two soils the estimated β values are

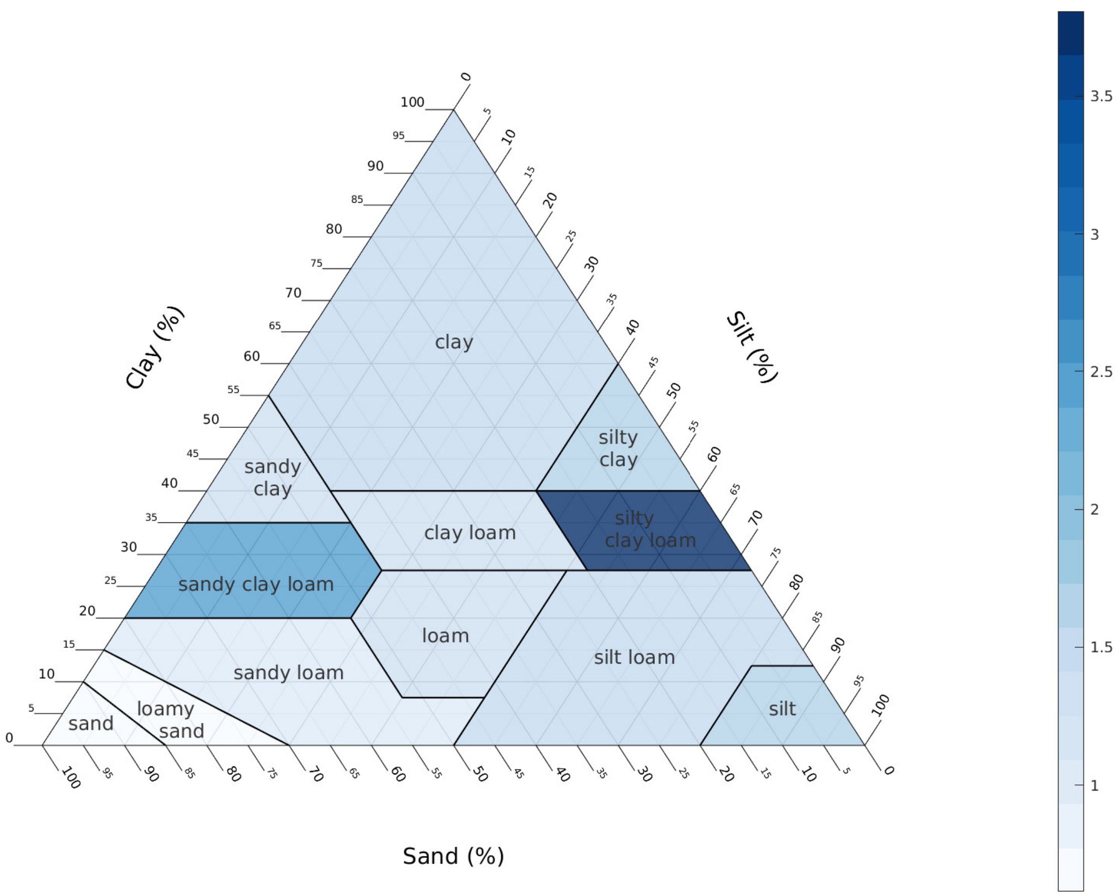

Figure 4.5 Inferred value of β on textural triangle.

greater than two. As we do not restrict the parameter β to 2, we see that for these two soils the β value is an outlier. In general it is noted that the β values for sandy soils are lower than the β values for clay. This confirms the hypothesis presented by Lassabatere et al. [2009] that finer soils have higher β values.

Lassabatere et al. [2009] has mentioned that the equations did not apply to the silty clay soil as the hydraulic properties did not fulfill the conditions for the quasi-exact formulation. Table 4.3 presents the correlation between the parameters S, K_s and β. For most of the soils we can see that the parameters are highly correlated with values being as high as 0.97. The DREAM posterior shows that all the parameters are positively correlated. Thus any change in one will be reflected in the values of the other parameters. The correlation between S and K_s make sense as the soil with finer texture will have lower sorptivity and hydraulic conductivity than the soil with coarser texture.

4.2 Results from Philip's equation

As the Philip's equation is widely used, the estimated parameters from Haverkamp's equation were then used to find out the c and the time up to which the Philip's equation is valid.

Figure 4.6 shows the contour plot of the BIC criterion for different sets of c and t_valid.

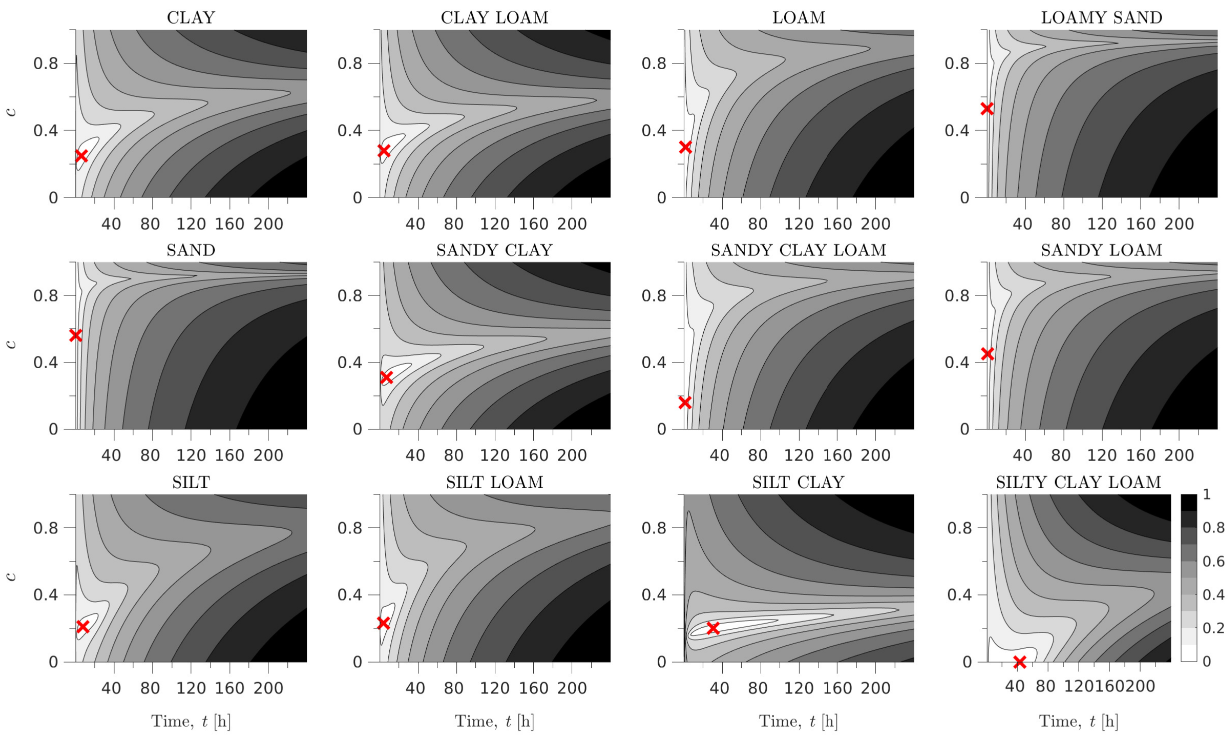

Figure 4.6 Contour plot for the Bayesian Information Criterion for the twelve USDA soils.

The contour plot gives clear optimum values. The red cross shows the optimized values of the$c$and t_valid which which indicate the minimum point of the BIC.

Figure 4.7 and 4.8 show the c_{Philip} and t_{valid} plotted on textural triangle. The c_{Philip} is higher for sand as compared to clay soil. Sand has higher infiltration in a given time period compared to the other soils so from the Philip's two term equation it can be inferred that the c_{Philip} would be higher. The first term, $S\sqrt{t}$, at the right-hand side of Eq. 1.1, dominates at early times when infiltration is largely determined by

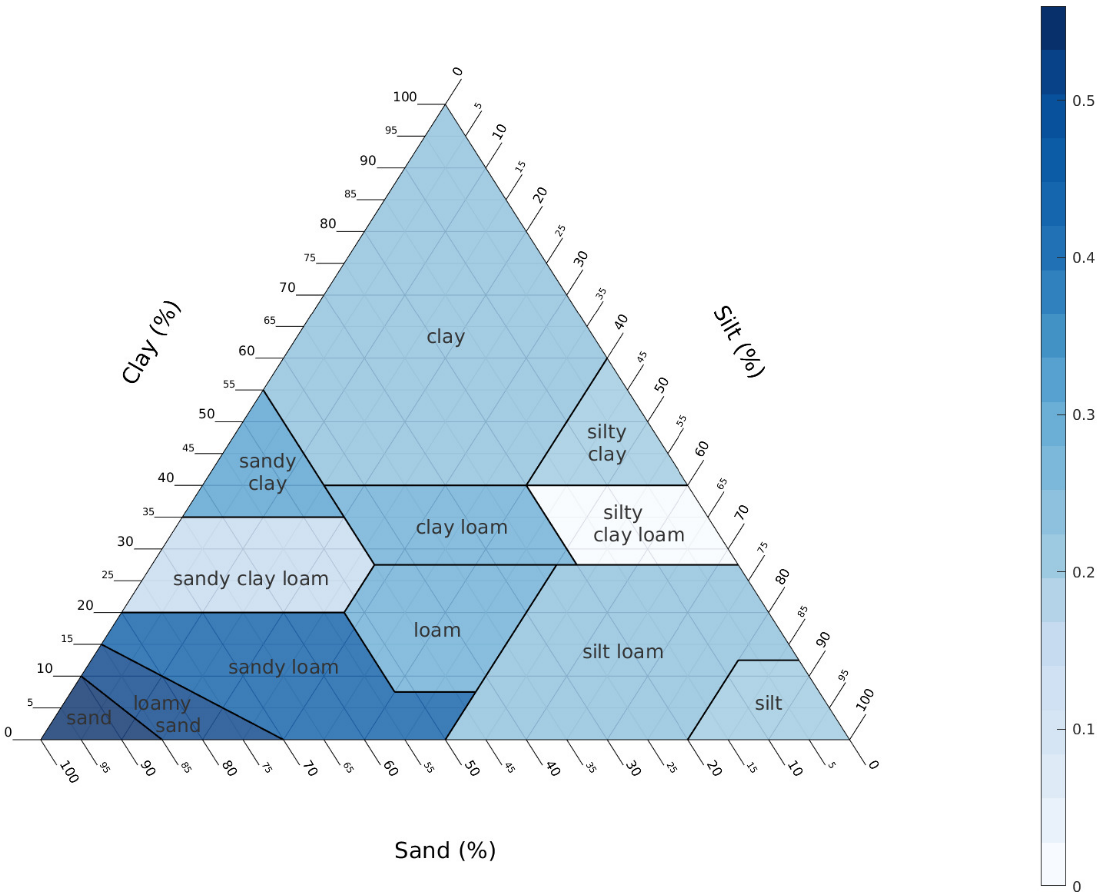

Figure 4.7 Optimized value of c_{Philip} on textural triangle for the twelve USDA soils.

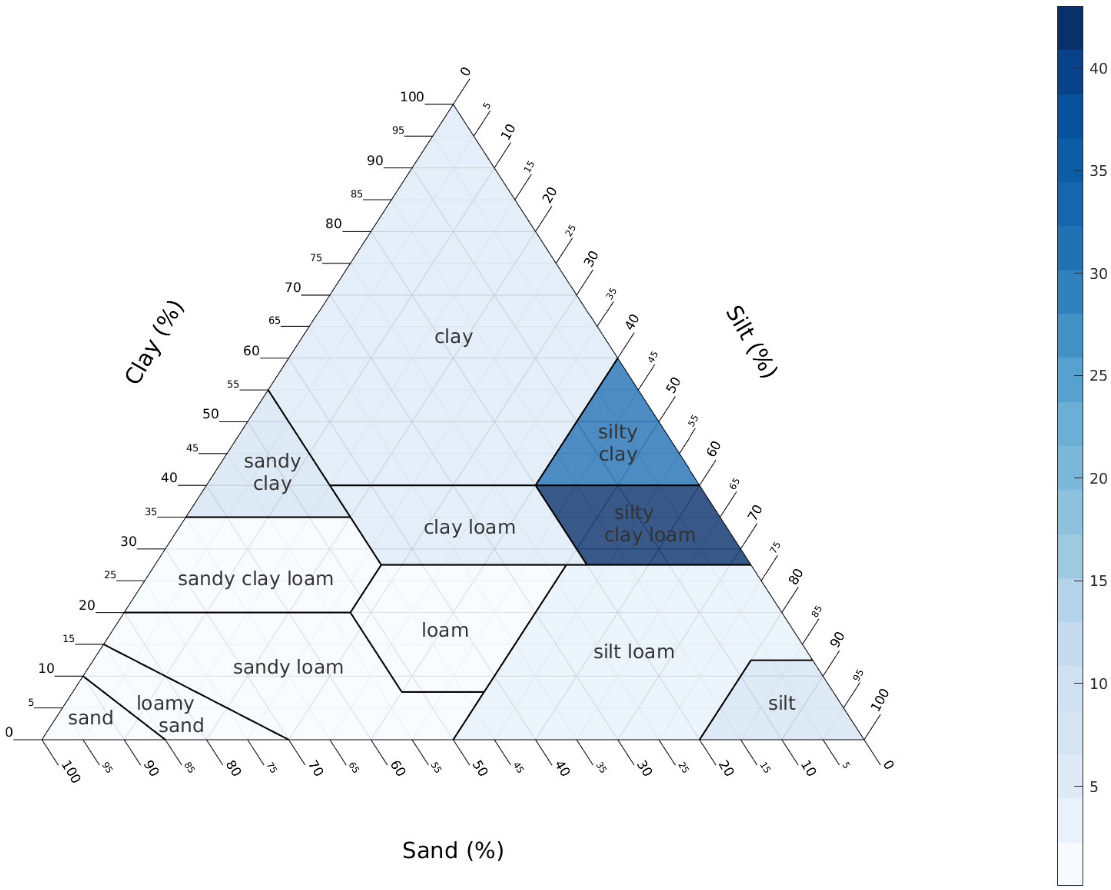

Figure 4.8 Optimized value of t_{valid} on textural triangle for the twelve USDA soils.

Table 4.4 Optimized results for the parameters for Philip's equation.

Parameters	c_{Philip}	t_{valid} hours	t_{char} hours
Clay	0.25	6.2032	26.0100
Clay loam	0.28	4.7842	31.1021
Loam	0.30	1.9950	4.4343
Loamy sand	0.53	0.2453	0.1805
Sand	0.56	0.1159	0.0962
Sandy clay	0.31	7.4915	42.2500
Sandy clay loam	0.16	1.1552	1.4918
Sandy loam	0.45	0.6383	0.7505
Silt	0.21	7.9703	28.7296
Silt loam	0.23	4.1833	13.4444
Silt clay	0.20	30.6717	306.2500
Silty clay loam	0	43.0141	55.1837

capillary forces. The second term, cK_st, increases steadily in magnitude as time elapses and the infiltration front progresses through the soil column. The time up to which the Philip's two term equation is valid will be shorter for sand as compared to clay soil.These inferences are verified by the textural triangle plots as they reflect the correlation between texture of soil and it's parameters

Table 4.4 lists the optimized values of c_{Philip} and t_{valid}. As we can see that c_{Philip} lies between zero and one and with most of them not going beyond one-third. Only the soil silty clay loam has a c value of zero. This is an exception as this would state that the hydraulic conductivity does not have an affect on the infiltration. Even though the hydraulic conductivity of this soil will be very low but it cannot be zero. So

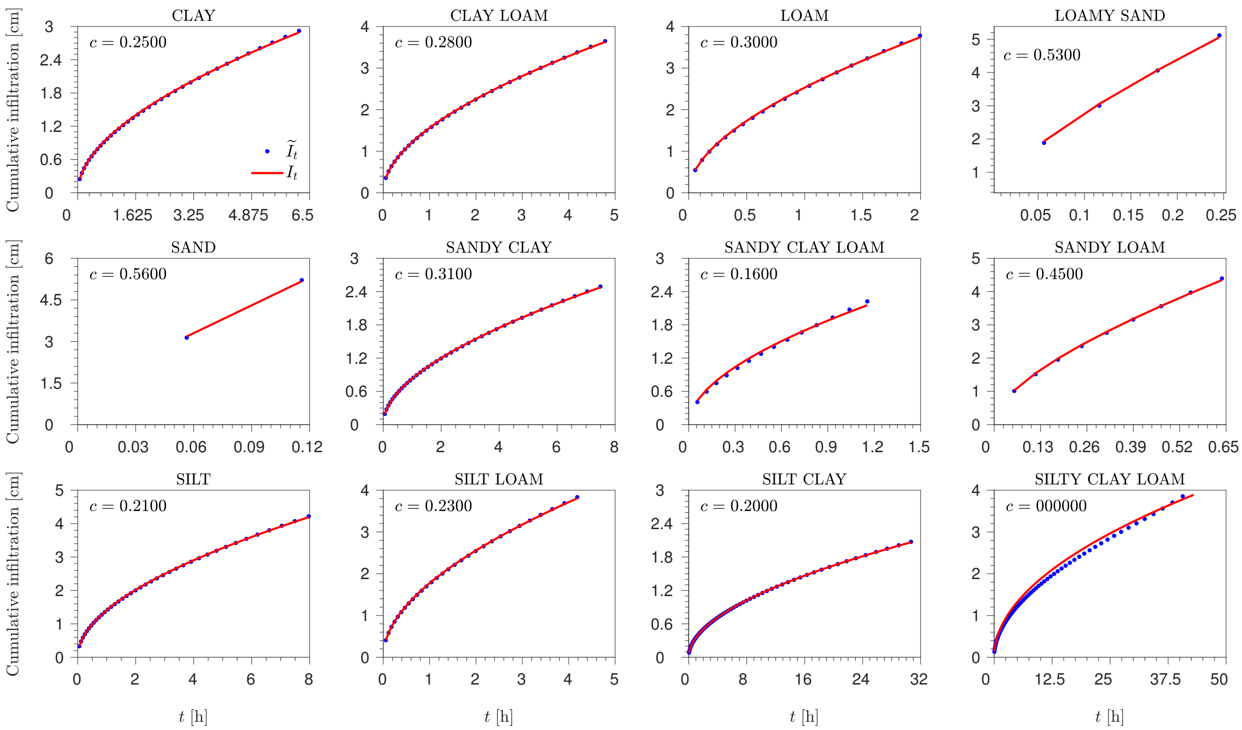

Figure 4.9 Comparison of true and two term Philip's equation using Haverkamp's S and K_s with optimized c values and t_valid

the method does not predict well for silty clay loam even though the estimation of hydraulic conductivity and sorptivity was accurate. The t_grav in the table is more than the t_valid for most of the soils as predicted by Philip [1957] that the two term equation would converge with $t \leq t_\mathrm{grav}$.

To test the equations we plot the "true" infiltration with the simulated infiltration values from the Philip's equation using the estimated values of S, K_s, c and t_valid. Figure 4.9 shows the predicted infiltration up to the valid time of the equation. As seen from the figures the observed infiltration values match the predicted infiltration

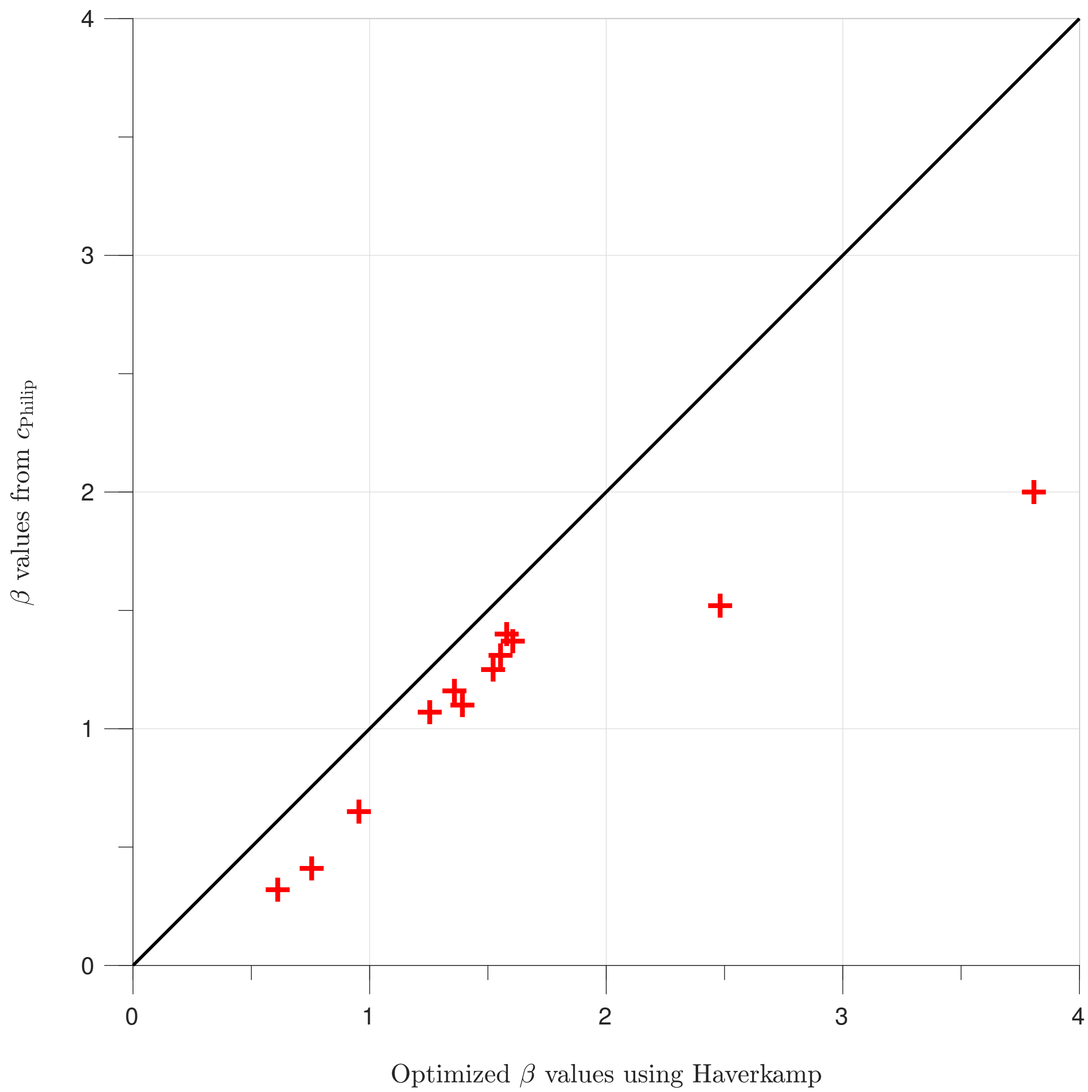

Figure 4.10 Scatter plot of β values optimized from Haverkamp's equation and from $\beta = 2 - 3 * c_{\text{Philip}}$

quite well up to the valid time. The only exception is the silty clay loam which overestimates for a brief period of time. We can see the discrepancy in the prediction of c value also as previously noted was coming out to be zero.

For further analysis on the β value, we compare the estimated value from DREAM and from the formula given by Moret-Fernández et al. [2017] Figure 4.10 when we know the value of c in the Philip's equation. Figure 4.10 shows the β estimated from the DREAM and the beta calculated from the optimized c values from the Philip's equation using the formula $c = (2\text{-}\beta)/3$ so $\beta = 2 - 3c$. The plot shows that the β from the c_{Philip} and DREAM have a linear relationship. The only two outliers are for sandy clay loam and silty clay loam soil. These two soils had β values more than two when the maximum beta value was set as 5. The outliers were tested by restricting β values at two. Both the values lie on the boundary (1.998 and 1.996) and the value of hydraulic conductivity and sorptivity were also affected because of correlation between parameters.

4.3 Summary and Conclusions

Estimation of the soil's sorptivity, S, and the saturated hydraulic conductivity, K_s , from infiltration experiments is typically obtained by fitting Philip [1957] two-term equation to measured infiltration curves. However, different estimation approaches may lead to different values of S and K_s for the same experimental infiltration data. There is strong correlation between S and K_s which makes it difficult for the estimation from the Philip's equation given that c and valid time for the Philip's equation are also unknown. Therefore, we used the quasi-exact formulation for cumulative infiltration [Haverkamp et al., 1994] combined with DREAM package[Vrugt, 2016] to estimate the S, K_s and β. We used HYDRUS-1D to simulate infiltration curves for soils with different textures ranging from sandy to clayey soils. We found that employing DREAM to estimate S and K_s from Haverkamp's equation provided accurate predictions of K_s and S when tested against numerically generated infiltration curves that were truncated to 5cm. The S and the K_s were also used for the Philip's equation to get the c and the time up to which the Philip's equation is valid. Then this Philip's equation was tested against the infiltration curves and we found that it provided accurate predictions for the cumulative infiltration. Further research needs to be done to get better estimates of β for sandy clay loam and silty clay loam soil as these two soils were the outliers for β value. Nevertheless the S and the K_s were well predicted for these soils. New efforts can be done in the direction of resolving the issues with the silty clay loam soil.

Appendix A

Matlab Codes

Code for evaluating Infiltration from Haverkamp's equation

```matlab
function [I] = Haverkamp_Eq3_s(t,x,maxiter)
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% This function evaluates Haverkamp's infiltration equation
%%
%% SYNOPSIS: [I] = Haverkamp_Eq3(t,x);
%%
%% Input   t          n x 1 vector with time in hours
%%         x          3 x 1 vector with S (cm h^(1/2)), K_s (cm h^-1)
%%                      and beta (-)
%%         max_iter   optional scalar with maximum number of iterations
%%
%% Output  I = cumulative infiltration as function of time, t
% %%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
% Default value of maximum iterations
if nargin < 3, maxiter = 20; end
% Parameter values input by user
S = x(1); K_s = x(2); beta = x(3);
% Default value of initial K
if numel(x) == 4, K_i = x(4); else, K_i = 0; end
```

```
dK = K_s - K_i;           % Compute delta K
n = numel(t);             % Number of elements of vector time
if dK <= 0, I = nan(n,1); return, end;  % If dK <= 0, return I = nan
I_0 = 0.2;                % Initial infiltration used for root finding
% Define Haverkamp equation
lhs = @(tj,dK,S,beta) (dK/S).^2 * ( 1 - beta ) * tj;
rhs = @(I,tj,dK,Ki,S,beta) dK*(I - Ki*tj)/S^2 ...
    - 1/2*log(1/beta * exp( (2*beta*dK*(I - Ki*tj))/S^2) ...
    + (beta - 1)/beta);
options = optimset('Display','off','FunValCheck','off'); % fzero options
% Dynamic part: Compute infiltration at each time,
for j = 1:n
    L = lhs(t(j),dK,S,beta);              % Compute LHS of Equation
    if j == 1 && t(j) == 0                % Infiltration when time is 0
        I(j,1) = 0;
    elseif j > 1 && t(j-1) == 0
        I(j,1) = fzero(@(z) rhs(z,t(j),dK,K_i,S,beta)...
            - L,I_0,options);
    else
        % First test that RHS is not Inf or imaginary number
        if j == 1
            R = rhs(I_0,t(j),dK,K_i,S,beta);      % Evaluating RHS
        elseif j == 2
            R = rhs(2*I(j-1,1),t(j),dK,K_i,S,beta);
        else
            R = rhs(2*I(j-1,1) - I(j-2,1),t(j),dK,K_i,S,beta);
        end
        if abs(R) < 1e10 %&& isreal(R)
            exitflag = 0; iter = 0;
            while ( exitflag ~= 1)
                [I(j,1),exitflag] = secant(@(z)...
                rhs(z,t(j),dK,K_i,S,beta) - L,I_0);
                iter = iter + 1;
                if iter > maxiter
                    I = 100*ones(n,1); % returning I if no root found
```

```
                    return
                end
            end
        else
            I = 100*ones(n,1); return
        end
    end
end
```

Code for finding root of a function

```
function [I,exitflag] = secant(fun,x0)
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%
%% This function calculates the root of equations using secant method
%%
%% SYNOPSIS: [I,exitflag] = secant(fun,x0);
%%
%% Input     fun      function of which the root is to be evaluated
%%           x0       starting point
%%
%% Output    I =          root of the function
%%           exitflag = check if the root is not finite or real
%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%%

n = 3;
x(n-1) = x0;   x(n-2) = x0+0.2;                 % set initial values
x(n) = ( x(n-2)*fun(x(n-1)) - x(n-1)*fun(x(n-2)) ) /...
    ( fun(x(n-1)) - fun(x(n-2)) );
exitflag = 1;
maxit = 20;                                     % maximum iterations
tol = 1e-10;                                    % setting tolerance
while  abs(fun((x(n)))) > tol && n < maxit
    n = n + 1;                                  % update counter
    % implementing secant method
```

```
    x(n) = ( x(n-2)*fun(x(n-1)) - x(n-1)*fun(x(n-2)) )...
        / ( fun(x(n-1)) - fun(x(n-2)) );
end
I = x(n);
% check the root for infinite or imaginary values
if ~isfinite(fun(x(n)))
    exitflag = 2;
elseif ~isreal(fun(x(n)))
    exitflag = 3;
elseif ~isfinite(x(n))
    exitflag = 4;
end
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